Toward Petascale Science and Engineering Simulation via PETSc

Satish Balay, Dinesh Kaushik, Mathew Knepley,
Barry Smith*, and Hong Zhang, Argonne National Laboratory

Summary

Partial differential equations (PDEs) are used to mathematically model phenomena in virtually all areas of science and engineering, from brain surgery to rocket science. We are developing the Portable, Extensible Toolkit for Scientific Computing (PETSc) to support high-performance petascale and terascale simulations based on PDEs. The parallel computing infrastructure and scalable numerical solvers in PETSc enable scientists and engineers to focus on their primary scientific interests, thereby reducing implementation costs and achieving results both faster and better.

Numerous ongoing application projects use various facets of PETSc. We highlight three recent projects. All have resulted in scientific and engineering advances; references may be found at our Web site: www.mcs.anl.gov/petsc/petsc-as/publications

Nuclear Energy. PETSc is extremely well poised to play a major role in GNEP (Global Nuclear Energy Partnership) simulations. These simulations are crucial for the design and optimization of the next generation of fission reactors. The PETSc solvers have been integrated into Argonne's UNIC neutronics code, allowing much larger simulations than previously possible. Next, we will parallelize this code using PETSc. The Idaho National Laboratory thermohydraulics package PCICE has already been parallelized by using the new Sieve technology in PETSc. Most important, these codes as well as others will be coupled by using the Empress framework being developed for GNEP. This will, for the first time, allow accurate, fully coupled, high-resolution simulations of fission reactors.

Environmental Science. Critical to the success of the Department of Energy's environmental stewardship is the development of numerical models for simulating subsurface flow and biogeochemical transport. These models provide tools for predicting the transport of subsurface contaminants and for investigating alternatives for site remediation. As scientific understanding of subsurface phenomena increases, multiphase flow and biogeochemical transport models have become more complex—simulating coupled heat transfer, multicontinuum-multiphase flow, and reactive multicomponent biogeochemical transport on higher-resolution 3D grids to account for small-scale spatial variability within the subsurface. The coupled solution of these nonlinear processes over a wide range of time and spatial scales presents a daunting computational challenge.

To address this challenge, researchers at PNNL, UIUC, and LANL have developed multiphase flow and biogeochemical transport capabilities that leverage the latest advances in computational science. Their

* Mathematics and Computer Science Division, (630) 252-9174, bsmith@mcs.anl.gov

transport model PARTRAN is founded on PETSc. In particular, PETSc provides the distributed arrays, linear and nonlinear solvers, preconditioners, and domain decomposition techniques needed to solve physically and biogeochemically complex subsurface problems. Indeed, the model has demonstrated commendable performance on several of the nation's top computing platforms (see Fig. 1).

Water Filtration: Polymer membranes have become the preferred method for filtering water, whether for removing particulates by mechanical separation or salt ions by reverse osmosis. At the same time, dwindling aquifers, depleted rivers, and changing weather patterns have exacerbated a crisis in water availability in the United States. To address this challenge, the U.S. Bureau of Reclamation is planning large-scale use of membrane filtration of sea water, at first to reach a level of purity acceptable for agricultural use, and later for municipal water supplies.

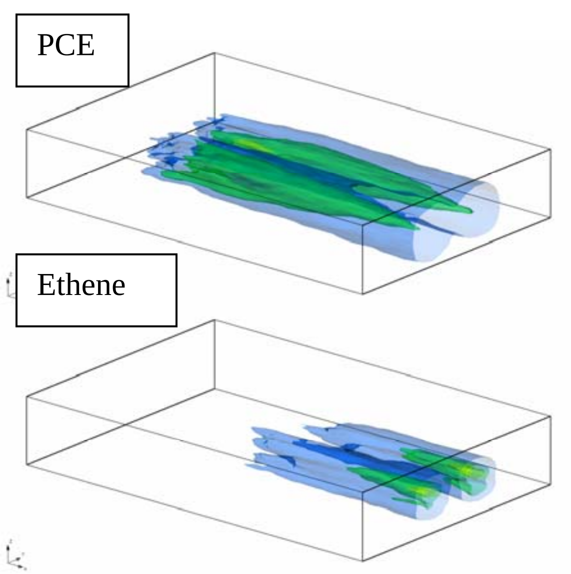

Figure 1. Isosurfaces of quasi-steady-state chlorinated ethene concentrations.

Polymer membranes for water filtration and desalination are usually made by phase inversion processes, primarily immersion precipitation. Immersion precipitation begins with a thin layer of polymer solution on a substrate, which is immersed into a liquid nonsolvent that diffuses into the solution layer; the solvent then diffuses out, causing the polymer to precipitate starting at the interface. Although the thermodynamics of polymer-solvent-nonsolvent systems are well understood, the kinetics of membrane formation are complicated, making this process more of an art than a science, with advances made by serendipitous tweaking of parameters and additives rather than by understanding the physical phenomena.
To gain deeper insight, the Powell group at MIT has used the phase field method to model the initial stages of phase decomposition and structure formation during immersion precipitation casting of a PVDF polymer membrane (see Fig. 2). The diffusion equations involve second derivatives of the chemical potential, which in turn have second derivatives of the composition—creating a fourth-order system of partial differential equations that PETSc is used to solve.

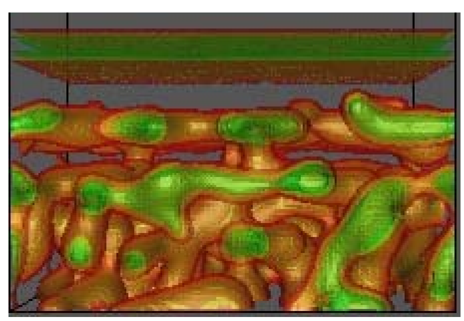

Figure 2 Details of calculated polymer membrane pore structure formation,

For further information on this subject contact:
Barry Smith
Argonne National Laboratory
Mathematics and Computer Science Division
petsc-maint@mcs.anl.gov
(630) 252- 9174